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EDUCATION AND JOBS

Assistant Chemist, Argonne National Laboratory, 2016-present

Argonne Scholar-Director's Fellow, Argonne National Laboratory, 2013 – 2016

Ph. D., Physical Chemistry, University of North Texas, 2009 – 2013

M. S. Study, Inorganic Chemistry, Shenyang University of Chemical Technology, China, 2007 – 2008

B. S., Chemistry, Shenyang University of Chemical Technology, China, 2003 – 2007

HONORS

Awards

- Chemical Computing Group (CCG) Research Excellence Award, 243th American Chemical Society (ACS) National Meeting, March 2012
- Outstanding International Graduate Student, University of North Texas, May 2013
- Poster Presentation Award, Southwest Theoretical Chemistry Conference, Oct. 2012
- First-place Presentation Award, 45th ACS Annual Meeting in Miniature DFW Section, April 2012
- Second-place Poster Presentation Award, Southwest Theoretical Chemistry Conference, Oct. 2010

Fellowships

- Director's Postdoctoral Fellowship, Argonne National Laboratory, 2013 - 2015
- Thesis and Dissertation Fellowship, University of North Texas, 2012 - 2013
- ACTC Fellowship, American Conference of Theoretical Chemistry, 2011

Scholarships

- Ed and Julia Hodges Memorial Scholarship for Outstanding Graduate Research, University of North Texas, June 2012
- Graduate Research Assistant Tuition Scholarship, University of North Texas, 2011 - 2012
- Graduate Student Travel Grant, University of North Texas, 2012
- Graduate Student Support Grants, University of North Texas, 2011
- Raupe Travel Grant, University of North Texas, 2011

RESEARCH

Assistant Chemist, Argonne National Laboratory (2016 – present)

Group Leader: Dr. Massimiliano Delferro

Argonne Scholar, Argonne National Laboratory (2013 – 2016)

Supervisor: Dr. Larry Curtiss

- Design of novel nanocatalysts for chemical and electrochemical CO₂ reduction and water splitting (BES program)

- Computational studies of catalytic biomass conversion to fuels using zeolites (EERE program, Computational Pyrolysis Consortium (CPC))
- Development of improved cathode materials for Li-ion batteries (EFRC program, Center for Electrochemical Energy Science (CEES))
- Development of single-site metal catalysts for alkane functionalization (BES program)
- Development of composite nanomaterials for Li-S batteries (Collaboration with Jun Lu and Khalil Amine at CSE, EERE program)
- Design of transition metal nanomaterial electrodes for CO₂ reduction and Li-O₂ batteries (Collaboration with Prof. Amin Salehi-Khojin University of Illinois at Chicago)
- Design of intermetallic metal nanoparticles for fuel cell applications (Collaboration with Prof. Wenyu Huang at Iowa State University)

Graduate Research Assistant, University of North Texas (2009 – 2013)

Research Advisor: Prof. Angela Wilson

Dissertation: “*Transition Metal Mediated C–O Bond Cleavage: From CO₂ Activation to Lignin Degradation*”

- CO₂ reactivity with homogeneous and heterogeneous transition metal catalysts
- Computational studies of catalytic lignin degradation using transition metal complexes
- Computational drug design (Collaboration with Reata Pharmaceuticals, Inc)
- Performance of density functional theory (DFT) methods on transition metal chemistry

Graduate Research Assistant, Shenyang University of Chemical Technology (2007 – 2008)

Research Advisor: Prof. Enjun Gao

- Synthesis of transition metal complexes with anti-cancer properties

Undergraduate Research Assistant, Shenyang University of Chemical Technology (2006 – 2007)

Research Advisor: Prof. Yongjie Chen

Thesis: “*Synthesis and Analysis of Rare Earth Element Containing LED Materials*”

- Synthesis and analysis of Eu²⁺, Dy²⁺, and Sm³⁺ containing inorganic calcium led compounds

PUBLICATIONS

1. H. Sohn, J. Camacho-Bunquin, R. R. Langeslay, P. A. A. Ignacio-de Leon, J. Niklas, O. G. Poluektov, **C. Liu**, J. G. Connell, D. Yang, A. J. Kropf, H. Kim, P. C Stair, M. Ferrandon and M. Delferro. Isolated, Well-defined Organovanadium(III) on Silica: Single-site Catalyst for Hydrogenation of Alkenes and Alkynes *Chem. Commun.*, **2017**, DOI: 10.1039/C7CC01876B
2. G. Tan, R. Xu, Z. Xing, Y. Yuan, J. Lu, J. Wen, **C. Liu**, L. Ma, C. Zhan, Q. Liu, T. Wu, Z. Jian, R. Shahbazian-Yassar, Y. Ren, D. J. Miller, L. A. Curtiss, X. Ji, K. Amine. Burning Lithium in CS₂ for High-performing Compact Li₂S-graphane Nanocapsules for Li-S Batteries. *Nat. Ener.* **2017**. DOI: 10.1038/nenergy.2017.90
3. B. Yang, * **C. Liu**, * A. Halder, E. Tyo, A.B.F. Martinson, S. Seifert, P. Zapol, L. A. Curtiss, S. Vajda. Copper Cluster Size Effect in Methanol Synthesis from CO₂. *J. Phys. Chem. C.* **2017**, 121(19), 10406. (* Equal Contributions)

- G. Tan, L. Chong, R. Amine, J. Lu, **C. Liu**, Y. Yuan, J. Wen, K. He, X. Bi, Y. Guo, H.-H. Wang, R. Shahbazian-Yassar, S. A. Hallaj, D. J. Miller, D. Liu, K. Amine. Toward Highly Efficient Electrocatalyst for Li–O₂ Batteries Using Biphasic N-Doping Cobalt@Graphene Multiple-Capsule Heterostructures. *Nano Lett.* **2017**, 17(5), 2959.
- Z. Qi, C. Xiao, **C. Liu**, T. W. Goh, L. Zhou, R. Maligal-Ganesh, Y. Pei, X. Li, L. A. Curtiss, and W. Huang. Sub-4 nm PtZn Intermetallic Nanoparticles for Enhanced Mass and Specific Activities in Catalytic Electro-Oxidation Reaction. *J. Am. Chem. Soc.* **2017**, 139 (13), 4762.
- J. Camacho-Bunquin, M. Ferrandon, U. Das, F. Dogan, **C. Liu**, C. Larsen, A. E. Platero-Prats, L. A. Curtiss, A. Hock, J. Miller, S. Nguyen, C. Marshall, M. Delferro, P. Stair. Supported Aluminum Catalysts for Olefin Hydrogenation. *ACS Catal.*, **2017**, 7 (1), 689.
- P. Abbasi, M. Asadi, **C. Liu**, S. S. Sharifi-Asl, A. Behranginia, B. Sayahpour, P. Zapol, R. S. Yassar, L. A. Curtiss, A. Salehi-Khojin. Tailoring the Edge Structure of Molybdenum Disulfide toward Electrocatalytic Reduction of Carbon Dioxide. *ACS Nano*, **2017**, 11 (1), 453.
- M. Asadi, K. Kim,* **C. Liu**,* V. A. Addepalli, P. Phillips, P. Abbasi, A. Behranginia, P. Yasaei, R. Haasch, P. Zapol, B. Kumar, R. F. Klie, J. Abiade, L. A. Curtiss, A. Salehi-Khojin. Nanostructured Transition Metal Dichalcogenide Electrocatalysts for CO₂ Reduction in Ionic Liquid. *Science*, **2016**, 353(6298), 467. (* Equal Contributions)
- M. Asadi, B. Kumar, **C. Liu**, P. Phillips, P. Yasaei, A. Behranginia, P. Zapol, R. F. Klie, L. A. Curtiss, A. Salehi-Khojin. A Molybdenum Disulfide/Ionic Liquid Co-catalyst for Lithium–Oxygen Batteries. *ACS Nano*, **2016**, 10 (2), 2167.
- A. Behranginia, M. Asadi, **C. Liu**, P. Yasaei, B. Kumar, P. Phillips, T. Foroozan, J. C. Waranius, J. Abiade, R. F. Klie, L. A. Curtiss, A. Salehi-Khojin. Highly Efficient Hydrogen Evolution Reaction Using Crystalline Layered Three Dimensional Molybdenum Disulfides Grown on Graphene Film. *Chem. Mater.*, **2016**, 28 (2), 549.
- C. Liu**, T. J. Evans, L. Cheng, M. R. Nimlos, C. Mukarakate, D. J. Robichaud, R. S. Assary, L. A. Curtiss. Catalytic Upgrading of Biomass-Derived Compounds via C-C Coupling Reactions: Furan and Acetaldehyde Reactions in HZSM-5. *J. Phys. Chem. C*. **2015**, 119 (42), 24025.
- C. Liu**, B. Yang, E. Tyo, S. Seifert, J. E. Ernst, B. von Issendorff, P. Zapol, S. Vajda, L. A. Curtiss. Carbon Dioxide Conversion to Methanol over Size-selected Cu₄ Clusters at Low Pressures. *J. Am. Chem. Soc.*, **2015**, 137 (27), 8676. (Reported by C&EN News, Chemeurope News, and Argonne News)
- C. Liu**, A. K. Wilson. Cleavage of the β-O-4 Linkage of Lignin using Group 8 Pincer Complexes: A DFT Study. *J. Mol. Catal. A: Chem.*, **2015**, 399, 33.
- C. Liu**, R. S. Assary, L. A. Curtiss. Investigation of Thermochemistry Associated with the Carbon–Carbon Coupling Reactions of Furan and Furfural Using ab Initio Methods. *J. Phys. Chem. A*, **2014**, 118 (25), 4392.
- C. Liu**, H. He, P. Zapol, L. A. Curtiss. Computational Studies of Electrochemical CO₂ Reduction on Subnanometer Transition Metal Clusters. *Phys. Chem. Chem. Phys.*, **2014**, 16, 26584. (Invited Paper)

16. M. R. Jones, **C. Liu**, A. K. Wilson. "Molecular Dynamics Studies of the Protein-Protein Interactions in Inhibitor of κ B Kinase- β " *J. Chem. Inf. Model.*, **2014**, 54 (2), 562. (**Graduate Student Mentoring Project**)
17. **C. Liu**, T. R. Cundari, A. K. Wilson. Periodic Trends in 3d Metal Mediated CO₂ Activation. *Applications of Molecular Modeling to Challenges in Clean Energy*. January 1, **2013**, 67. (**Invited Book Chapter**)
18. **C. Liu**, C. Peterson, A. K. Wilson. C-O Bond Cleavage of Dimethyl Ether by Transition Metal Ions: A Systematic Study on Catalytic Properties of Metals and Performance of DFT Functionals. *J. Phys. Chem. A*, **2013**, 117 (24), 5140.
19. **C. Liu**, T. R. Cundari, A. K. Wilson. Reduction of CO₂ to CO on Transition Metal Surfaces: In Comparison with Homogeneous Catalysis. *J. Phys. Chem. C*, **2012**, 116 (9), 5681.
20. **C. Liu**, T. R. Cundari, A. K. Wilson. Reaction Mechanism of the Reverse Water-gas Shift Reaction Using First-row Middle Transition Metal Catalysts L'M(M: Fe, Mn, Co): A Computational Study. *Inorg. Chem.*, **2011**, 50 (18), 8782.
21. **C. Liu**, L. Munjanja, T. R. Cundari, A. K. Wilson. Theoretical Studies on the Catalysis of the Reverse Water Gas Shift Reaction Using First-row Transition Metal β -diketiminato Complexes. *J. Phys. Chem. A*. **2010**, 114, 6207. (**Undergraduate Student Mentoring Project**)
22. E. Gao, **C. Liu**, M. Zhu, H. Lin, Q. Wu, L. Liu. Current Development of Pd(II) Complexes as Potential Antitumor Agents. *Anticancer Agents Med. Chem.* **2009**, 9(3), 356.
23. E. Gao, Q. Wu, **C. Liu**, F. Liu, H. Liu. Syntheses and DNA-Binding Study of the Zinc (II) Complex with 2,5-Thiophenedicarboxylic Acid. *J. Chin. Clin. Med.* **2008**, 3(8), 442.

LEADERSHIP AND SERVICE

- Reviewer for multiple scientific journals including JACS, ACS Catalysis, Nano Energy, JPC, etc.
- Outstanding Reviewer for the Journal of Computational and Theoretical Chemistry, 2015
- Oral Presentation Session Chair in COMP division, 247th, 248th and 249th ACS National Meetings
- Judge for the Physical Chemistry Poster Award, 247th ACS National Meeting

SELECTED PRESENTATIONS

1. "Computational Studies of Electrochemical Reduction of CO₂ to CO using Transition Metal Dichalcogenide Nanoflakes", 253rd ACS National Meeting, April 2017.
2. "Trends of SiO₂ Supported Single-site Catalysts for Alkene Hydrogenation based on Combined DFT and Experimental Studies", 253rd ACS National Meeting, April 2017.
3. "Computational Studies of Doping and Dissolution in Lithium Transition Metal Oxides", 2016 MRS Spring Meeting & Exhibit, March 2016.
4. "Computational Studies of Chemical and Electrochemical CO₂ Reduction: From Metals Surfaces and Metal Clusters to Semiconductors", 250th ACS National Meeting, August 2015.

5. "In Silico Zeolite Catalyzed Carbon-Carbon Coupling Reactions for Furan Upgrading", 249th ACS National Meeting, March 2015. (**Invited Talk**)
6. "Electronchemical Reduction of CO₂ to Fuels using Supported Transition Metal Clusters: Comparison with Gas-Phase Reactions" 248th ACS National Meeting, August 2014.
7. "Computational Studies of C-C Coupling to Increase the Carbon Content of Furans with Zeolite Catalysts" 247th ACS National Meeting, March 2014.
8. "Transition Metal Catalyst Mediated C-O Bond Activation of the β -O-4 Linkage of Lignin", 245th ACS National Meeting, April 2013.
9. "C-O Bond Cleavage Using Transition Metal Catalysts: From Dimethyl Ether Activation To Lignin Degradation", 245th ACS National Meeting, April 2013.
10. "Transition Metal Catalysts Mediated C-O Bond Cleavage of β -O-4 Linkage of Lignin", Southwest Theoretical Chemistry Conference, October 2012.
11. "Computational Studies of CO₂ Activation and Conversion using 3d Transition Metal Catalysts", International Conference of Quantum Chemistry, June 2012.
12. "Computational Studies on Transition Metal Catalysts Mediated CO₂ Activation", 45th ACS Meeting in Miniature DFW Section, April 2012.
13. "Computational Studies on CO₂ Activation using Transition Metal Catalysts: In Consideration of Homogeneous and Heterogeneous Catalysis", 243th ACS National Meeting, March 2012.
14. "DFT Studies on CO₂ Activation using Homogeneous and Heterogeneous Transition Metal Catalysts", 24th Austin Symposium on Molecular Structure and Dynamics at Dallas, March 2012.
15. "CO₂ Activation by Transition Metal Catalysts: In Consideration of Homogeneous and Heterogeneous Catalysis", 2011 Southwest Theoretical Chemistry Conference, October 2011.
16. "CO₂ Reduction on Transition Metal Surfaces: A Computational Study", American Conference of Theoretical Chemistry, July 2011.
17. "Reaction Mechanism of the Reverse Water-gas Shift Reaction Using Transition Metal Catalysts L'M (L': β -diketiminato, M: Fe, Mn, Co): A Computational Study", 44th ACS Annual Meeting in Miniature DFW Section, April 2011.
18. "Computational Studies of CO₂ Activation and Conversion Using Transition Metal β -diketiminato Complexes", Southwest Theoretical Chemistry Conference, October 2010.
19. "Thermodynamics and Kinetics of CO₂ Activation using Middle Transition Metal Complexes", The Chemistry Centennial Celebration, University of North Texas, October 2010.
20. "Theoretical Studies of the Activation of Carbon Dioxide Using Transition Metal β -diketiminato Complexes", 240th ACS National Meeting, August 2010.

21. “Modeled Mechanism of the Reverse Water Gas Shift Reaction Using Transition Metal catalysts”, ACS Summer School on Green Chemistry and Sustainable Energy, July 2010.
22. “Theoretical Studies on the Catalysis of the Reverse Water Gas Shift Reaction Using Transition Metal β -diketiminato Complexes”, 43rd Annual Meeting in Miniature, April 2010.
23. “ β -diketiminato catalysts and their potential role in CO₂ activation”, 239th ACS National Meeting, March 2010.